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Polymorphism and a Phase Transition in K3Yb(PO4)2

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Alkali lanthanide double phosphates have been studied for use as long-wavelength scintillators for γ-ray detection using Si photodiodes. These compounds exhibit layered crystal structures. Details of the crystal symmetry depend on the relative sizes of the lanthanide and alkali metals. Single-crystal x-ray diffraction (XRD) and powder neutron diffraction (PND) have been used to study the structure at room temperature. $K_3Yb(PO_4)_2$ crystallizes with a monoclinic unit cell, space group $P2_1/m$. The Yb ion is six-coordinated to the oxygen atoms of the phosphate groups with uint cell parameters a = 7.372(1), b = 5.589(1), c = 9.292(2) Å and β = 91.03°. The Yb ion is seven coordinated with a slightly distorted capped trigonal pism (CTP) geometry. A high temperature phase was characterized using powder neutron diffraction and synchotron powder analysis. The phase transition occurs at 120°C with a transformation to the hexagonal P-3 space group symettry with a coordination reduction to six that is confirmed using EXAFS. This new structure is isostructural with the room-temperature form of $K_3Lu(PO_4)_2$. High temperature PND and high temperature powder XRD have been used to study the thermal expansion of $K_3Yb(PO_4)_2$ and indicate a large thermal expansion anisotropy.

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